Lattice QCD computing at BNL

Ruth Van de Water, Taku Izubuchi

DOE HEP Computing Review
February 9, 2011

Who we are

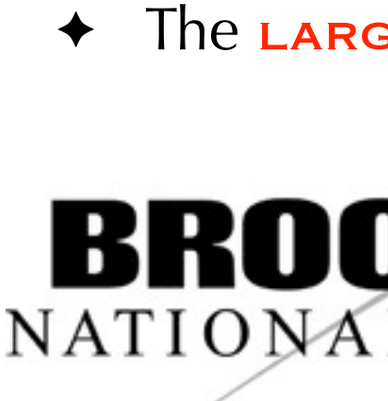
- The LARGEST COLLECTION OF LATTICE GAUGE THEORISTS IN THE UNITED STATES

BROOKHAVEN NATIONAL LABORATORY

High-energy theory
Mike Creutz
Taku Izubuchi
Chulwoo Jung
Amarjit Soni
Ruth Van de Water

Nuclear theory
Frithjof Karsch
Swagato Mukherjee
Peter Petresky

collaborators at Columbia University
Norman Christ
Bob Mawhinney



RBRC Research Center
(Yasumichi Aoki)
T.I.
Shigemi Ohta

collaborator at the University of Connecticut
Tom Blum

APS

collaborator at the American Physical Society
Urs Heller

- ... plus several postdocs and graduate students at BNL, Columbia, and UConn
  (about 10 PhD students are working, about 20 thesis are produced for last 6 years)

- We work with the RBC, UKQCD, hotQCD, and MILC Collaborations, which have members at other institutions around the U.S. and Europe

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Will focus on the work of the high-energy theory group in this presentation

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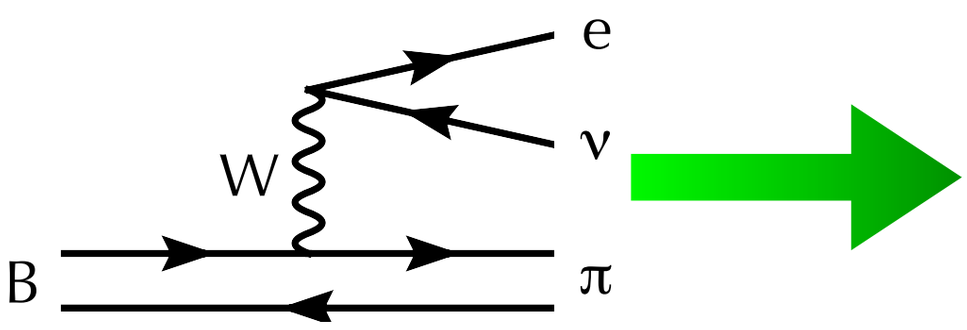
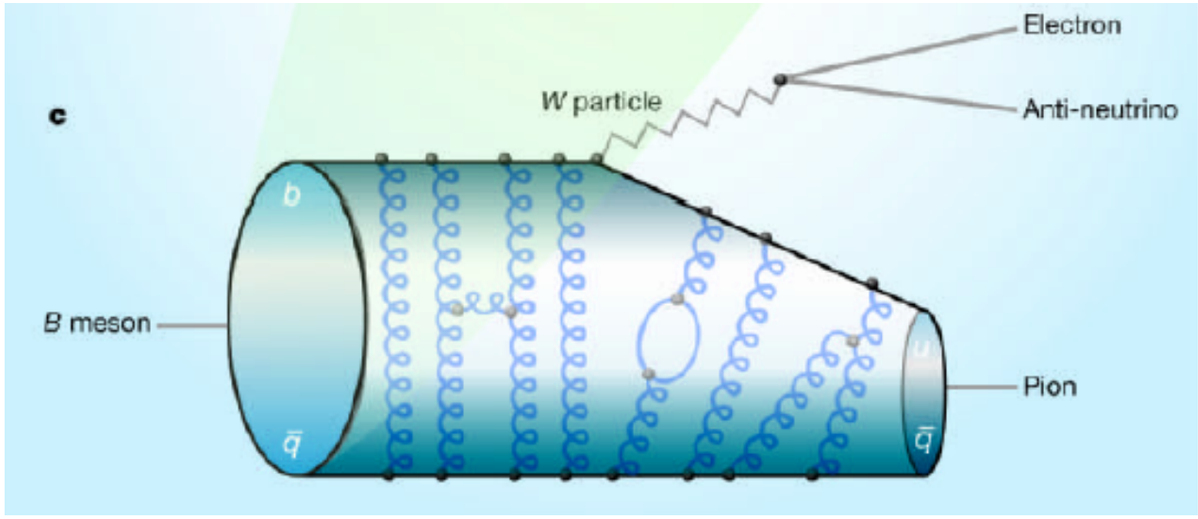
What we do: flavor physics phenomenology

- Experiments have been pouring out data to pin down the CKM matrix elements (which are fundamental parameters of the Standard Model) but lattice calculations are needed to interpret many of their results

  - Schematically, **EXPT. = CKM × LATTICE**

- In order to accurately describe weak interactions involving quarks, must include effects of confining quarks into hadrons:





- Typically absorb nonperturbative QCD effects into quantities such as decay constants, form factors, and bag-parameters which we must compute in lattice QCD

- **Precise lattice QCD calculations of hadronic weak matrix elements are critical to maximize the scientific output of the experimental high-energy physics program**

Scientific strengths

- Members of the HET group at BNL are among the world leaders in lattice QCD calculations relevant for kaon physics phenomenology
- Due in large part to the use of the domain-wall fermion formulation for the light up, down, and strange quarks
  - Domain-wall quarks have an approximate chiral symmetry on the lattice that makes them particularly well-suited to weak matrix element calculations
  - Have enabled the reduction of key systematic errors such as those from the chiral extrapolation and renormalization
- Members of BNL HET pioneered the use of domain-wall quarks in lattice QCD calculations in 1997, and included the effects of all three light quarks (u,d, & s) in the vacuum polarization in 2005
- Because domain-wall fermions are one of the most computationally intensive lattice formulations, **use of dedicated, high-performance computing resources was key to this scientific breakthrough**

Recent accomplishments

- World's best 2+1 flavor lattice calculation of kaon mixing parameter B_K

Continuum Limit of B_K from 2+1 Flavor Domain Wall QCD

Y. Aoki,[1,2] R. Arthur,[3] T. Blum,[4] P.A. Boyle,[3] D. Brömmel,[5,6] N.H. Christ,[7] C. Dawson,[8] T. Izubuchi,[1,9] C. Jung,[9] C. Kelly,[3] R.D. Kenway,[3] M. Lightman,[7] R.D. Mawhinney,[7] Shigemi Ohta (太田滋生),[10,11,1] C.T. Sachrajda,[5] E.E. Scholz,[12] A. Soni,[9] C. Sturm,[9,13] J. Wennekers,[3] and R. Zhou[4,14]

(RBC and UKQCD Collaborations)

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Regular Article - Theoretical Physics

- World's best 2+1 flavor calculation of the $K \to \pi l \nu$ form factor; leads to single best determination of CKM element $|V_{us}|$

$K \to \pi$ form factors with reduced model dependence

The RBC-UKQCD Collaboration

PHYSICAL REVIEW D **82,** 014505 (2010)

Neutral *B*-meson mixing from unquenched lattice QCD with domain-wall light quarks and static *b* quarks

C. Albertus,[1,*] Y. Aoki,[2] P. A. Boyle,[3] N. H. Christ,[4] T. T. Dumitrescu,[4,†] J. M. Flynn,[1] T. Ishikawa,[2,‡] T. Izubuchi,[2,3] O. Loktik,[4] C. T. Sachrajda,[1] A. Soni,[5] R. S. Van de Water,[3] J. Wennekers,[3,§,‖] and O. Witzel[5]

(RBC and UKQCD Collaborations)

- First calculation of B-mixing matrix elements with dynamical domain-wall quarks

Current computational resources

Dedicated lattice hardware at BNL: QCDOC

- Design, construction, and efficient coding of massively parallel computers a critical ingredient in the success of BNL's lattice field theory program

- Members of BNL HET (with collaborators at RBRC and Columbia) **designed the QCDOC specifically for lattice calculations**

  - Precursor to the IBM Blue Gene series which is now widely used in all areas of scientific computing

- BNL hosts two QCDOC systems:

  - 10 TFlop peak machine owned by RBRC & 10 TFlop peak machine owned by USQCD

  - RBRC-owned machine used solely by members or the RIKEN-BNL-Columbia (RBC) collaboration; valuable in-house resource for experimental ideas that has led to many essential breakthroughs

  - USQCD-owned machine purchased with DOE funds (through ASCR) and shared by U.S. lattice QCD community; time allocated by scientific programming committee

- BNL provides power, cooling, space, and hardware support staff for both systems

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The USQCD Collaboration

- Coordinated effort to design software and create dedicated hardware resources to facilitate lattice gauge theory calculations
  - Membership available to all U.S. lattice gauge theorists
  - Software development funded through a DOE SciDAC grant
  - Hardware purchased through the LQCD project funded by the Office of Science's high-energy and nuclear physics programs

- **Computing resources available to all members and peer-allocated annually** by the Scientific Program Committee
- BNL theorists are members of both the Executive Committee (Frithjof Karsch) and Scientific Program Committee (Taku Izubuchi and Frithjof Karsch, chair)

USQCD computing resources

- **Commodity clusters deployed at Fermilab and Jefferson Lab**: ~20 TFlops sustained
  dedicated to lattice gauge theory

  - Fermilab and JLab provide power and space
  - Some staff to support operations is funded by the LQCD project
  - Fermilab cluster used by members of BNL HET for analysis

- **Intrepid**: 557 TFlop peak IBM Blue Gene/P at Argonne National Lab

  - One of the largest 2011 INCITE allocation on Intrepid awarded to USQCD (50 M proc.-hrs.)
  - Distribution of computing time among members decided by USQCD Scientific Program Committee
  - Used by members of BNL HET for both domain-wall configuration generation and analysis

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42% of BNL HET computing usage

Other computing resources

- **New York Blue**: 100 TFlop peak IBM Blue Gene/L and 25 TFlop peak BG/P housed at BNL
  - Owned by Stony Brook University (purchased by NY state) and housed at BNL
  - Computing time allocated by New York Center for Computational Sciences and shared among users at BNL, Stony Brook, ...

- Also use time at **RICC** (Riken Integrated Cluster of Clusters) in Japan

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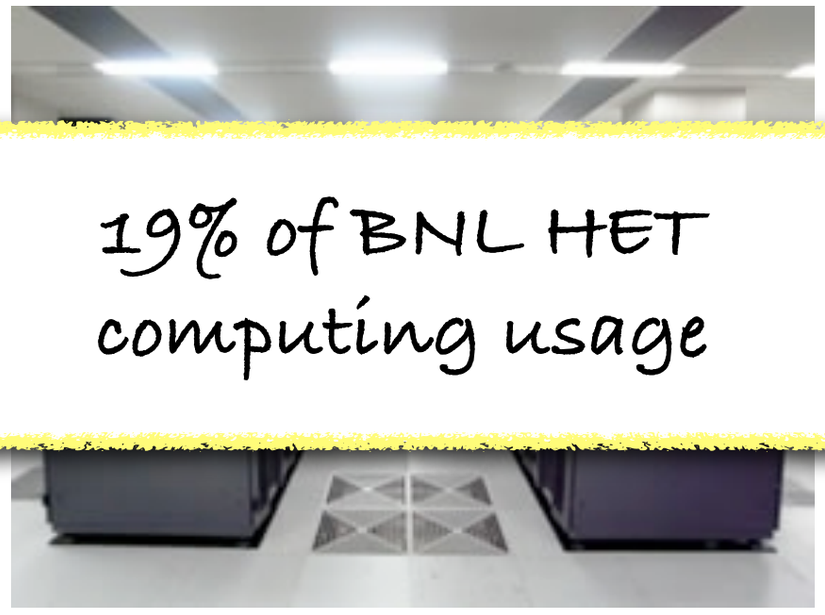

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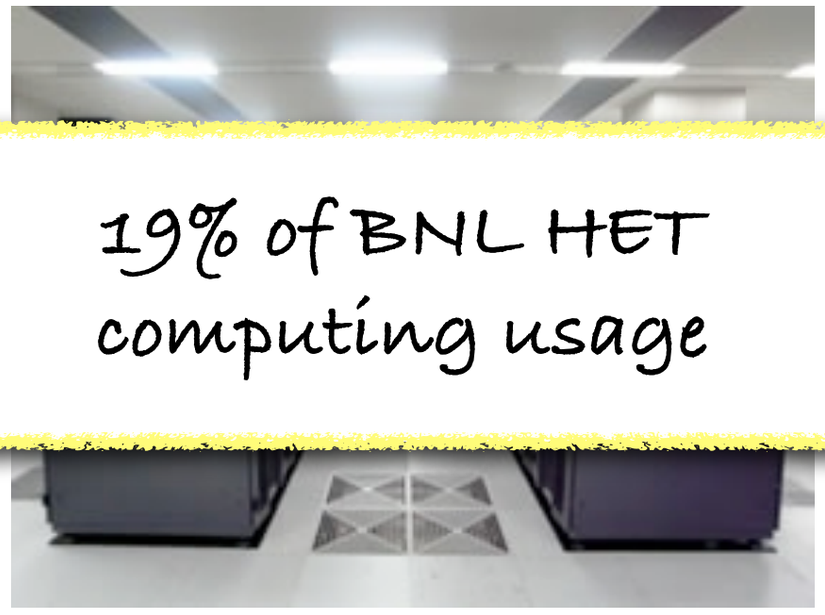


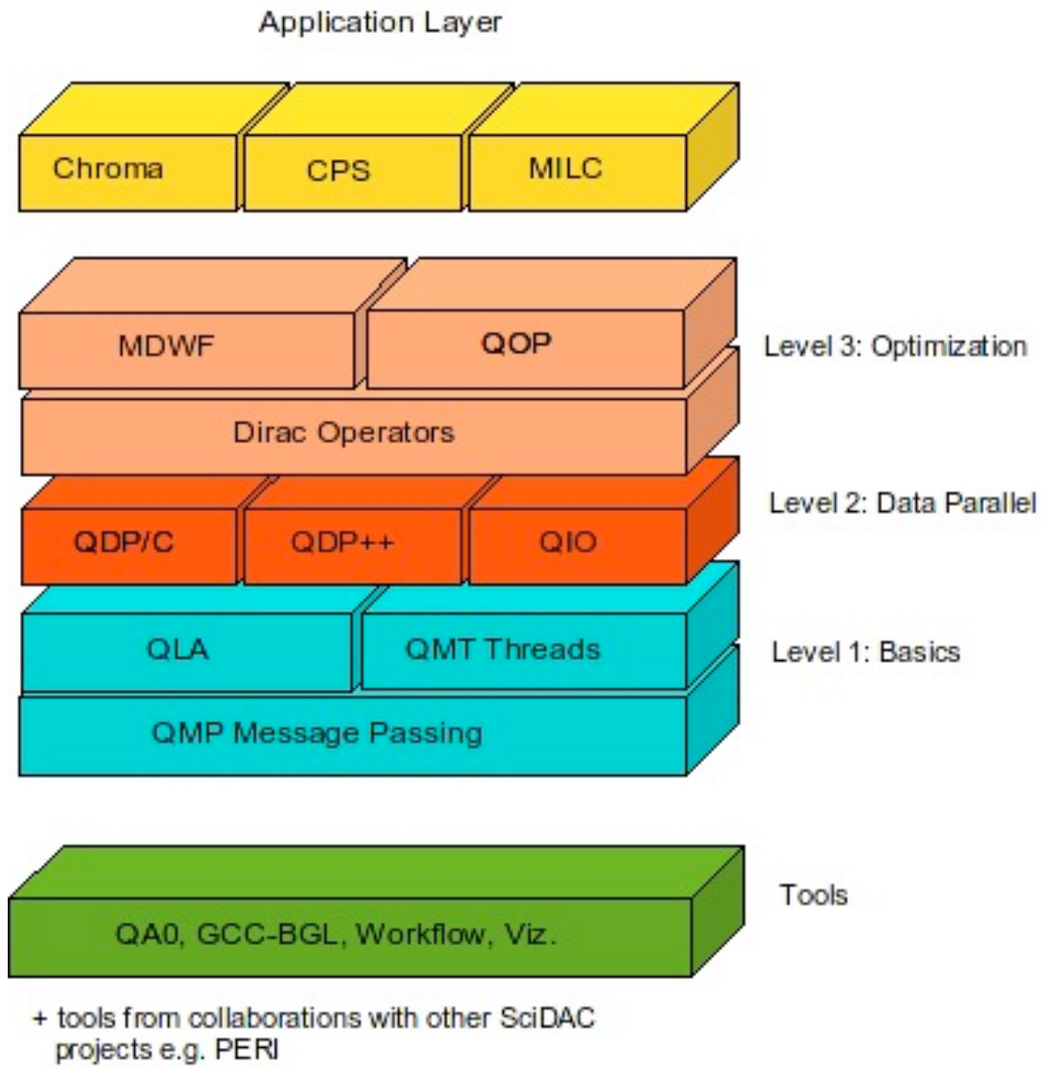
19% of BNL HET computing usage

Total BNL HET computing usage for 2010:
14.7 TFlop-years
(sustained)

Lattice gauge theory software

- Under a DOE SciDAC grant, USQCD has developed **lattice gauge theory software enabling efficient computing across a variety of architectures** including custom facilities and commodity clusters

- Three independent high-level frameworks (Chroma, CPS++, and MILC) **allow new users to start substantial projects** with minimal coding experience and overhead



- Members of the BNL HET use all three software systems, but are primarily involved in the development of CPS++, a C++-based lattice QCD library supported for use on the QCDOC, IBM BlueGene series, and PC clusters

- Funding from SciDAC grant **provides the salary of one postdoc and one staff member in the BNL HET group** specifically to work on software for the USQCD collaboration

Future plans

Scientific goals: I

KAONS

- Over the next three years, will continue effort in kaon physics, with the **key goal of obtaining the first calculation of $K \to \pi\pi$ matrix elements and the direct CP violation parameter ε'/ε including three dynamical quarks with all sources of systematic uncertainty under control**
  - Occur via 1-loop penguin diagrams in the Standard Model, so are particularly sensitive to new physics contributions
  - Precise experimental measurements already available, but are waiting for sufficiently reliable lattice QCD calculations to search for new physics in these channels

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B-PHYSICS

- Currently developing a program in B-meson physics
  - Initial focus on simple (but still phenomenologically interesting) lattice quantities such as **decay constants and mixing amplitudes** to obtain the CKM matrix elements $|V_{td}|/|V_{ts}|$
  - Will then turn attention to form factors of semileptonic decays such as $B \to \pi l \upsilon$ and $B \to D^* l \upsilon$, which are needed for $|V_{ub}|$ and $|V_{cb}|$ from exclusive decay channels

Scientific goals: II

Other areas

- Maintain intellectual vitality by pursuing more challenging exploratory calculations:
  - Hadronic light-by-light contribution to the muon's anomalous magnetic moment
  - Proton and neutron electric dipole moments
  - ...

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Proposed research plan is computationally demanding, and will require new petascale computing resources...

Successor to the QCDOC: IBM BG/Q

- Members of BNL HET collaborating with researchers at RIKEN, Columbia, Edinburgh, and IBM Watson Laboratory to design the next generation IBM BlueGene machine, the BG/Q
- In late 2011 **two 200 TFlop peak racks of a prototype BG/Q will be installed at BNL** in the location currently housing the QCDOC
  - One rack purchased by RBRC for the use of the RBC collaboration
  - Other purchased by BNL for the use of the entire laboratory
- **BNL will pay for space, power, cooling, and support staff for both racks**
  - Replacements for current machines, so do not require new infrastructure
- Some **fraction of computing time on the BNL-owned rack will be given to the USQCD collaboration** for code development
  - Will enable USQCD to be ready to run at Argonne when the 10 PFlop BG/Q "Mira" is installed in 2012

USQCD hardware at BNL

- Under the DOE LQCD-ext project, USQCD expects to purchase substantial hardware each year to be deployed among BNL, Fermilab, and JLab for use by members of the collaboration
  - Specific hardware will be chosen each year to provide the most cost-effective means to achieve the physics goals of the collaboration
  - Likely that in 2012 and 2013 the BG/Q will be the appropriate choice
  - If so, **BNL expects to host the USQCD machine**

Summary and outlook

- BNL HET group has **both technical expertise in numerical lattice QCD simulations and broad knowledge of flavor phenomenology in the quark sector**
- Play key role in developing new hardware and software for lattice calculations
  - Allowed RBRC and BNL to obtain two racks of prototype BG/Q at well below the commercial price
- Attacking several of the most important weak-matrix elements for CKM phenomenology
  - Well-established program in kaon physics has lead to the current best calculations of the $K \to \pi l \nu$ form factor and neutral-kaon mixing parameter B_K
  - Now turning our attention to the more challenging target of $K \to \pi\pi$ decay and developing a B- and D-meson physics program using domain-wall light quarks
- Physics program is computationally demanding, but are procuring hardware and developing software to enable its successful completion
- Lattice QCD at BNL is poised to play a key role in discovering new physics in the flavor sector!